



CINT Report to BES/SUFD
April 7, 2017

High-Impact Science Highlights (Slides and original papers are attached)

Category: *Enablers*. Can we engineer polymers to have superior electronic and structural properties? Polymer nanocomposites that integrate nanoparticles into polymer melts often possess superior mechanical, thermal, optical, or electrical properties in comparison with pure polymeric materials. Fabrication and processing of polymer nanocomposites require a good understanding of their viscoelastic behavior. Central to the viscoelasticity of polymer nanocomposites is the coupling

between the motion of nanoparticles and the relaxation dynamics of matrix chains. For long entangled polymers, this dynamic coupling depends strongly on the nanoparticle diameter compared to the entanglement mesh of the polymer matrix together with the polymer architecture. In “Nanoparticle Motion in Entangled Melts of Linear and Nonconcatenated Ring Polymers” (see attached files [Macro_Ge_April2017.pdf](#) and [Macro_Ge_April2017.pptx](#)) the authors used large-scale molecular dynamics simulations to compare the motion of nanoparticles in melts of linear and ring polymers. This comparison provides a paradigm for the effects of polymer architecture on the dynamical coupling between nanoparticles and polymers in nanocomposites. They show that for nanoparticles larger than the entanglement mesh size of the polymer, their motion is strongly suppressed for both linear and ring polymers, giving rise to subdiffusive motion of the nanoparticles prior to the onset of the long-time Fickian diffusion. However, the degree of suppression is much less in ring polymers compared to linear polymers due to the effect that chain ends have on the degree of polymer entanglements. These results demonstrate the role of polymer architecture in the dynamical coupling between nanoparticles and polymers in nanocomposites.

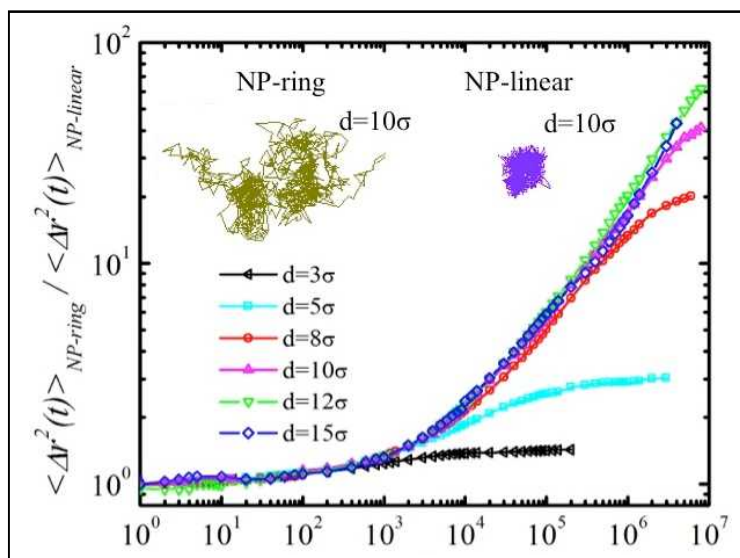


Figure 1: Ratio of the mean squared displacement of NPs in melt of ring and linear polymers. Trajectory of a NP in melt of ring polymers (dark yellow line) and linear chains (violet line) for a time period of 10^5 times the characteristic time of the polymer, τ .

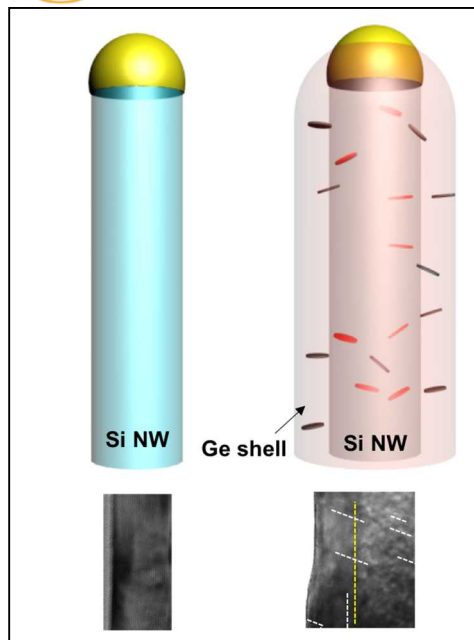


Figure 2: Defect-free single crystalline Si nanowire generates structural defects from stress when Ge shell becomes thicker.

Category: *Enablers and cross-cutting.* Can we increase Si nanowire (NW) anode performance for use in Lithium ion batteries? Lithium ion battery anodes made from nanowire heterostructures consisting of a Si core and Ge shell show better capacity at fast charging rates compared to pure Si nanowires, but suffer from defect propagation, limiting overall performance. However, it is unclear where do the defects originally come from - the wire or the shell? In “Strain-induced structural defects and their effects on the electrochemical performances of silicon core/germanium shell nanowire heterostructures” (see attached files [Nanoscale_Lin_April2017.pdf](#) and [Nanoscale_Lin_April2017.pptx](#)), the authors perform an integrated study of both structural characterization and electrochemical performance to discover the actual root cause. Their work showed that radial heteroepitaxial

shell growth induces structural defects in the core nanowires (NWs), relaxing strain in both the core and shell regions. The induced structural defects then affect the electrochemical performance of the combined core/shell NW heterostructure. The concept of crossover defects in these radial NW heterostructures provides a new tunable parameter for design and optimization of these devices for use in electrical energy storage applications. In addition, the concept becomes crucial in applications such as electronic/photonic devices based on three-dimensional architectures. The observations from this research can serve as a framework or guideline for the design of heterostructures at the nano- and microscale.

Scientific Leadership:

- I. The CINT Scientific Advisory Committee (SAC) recently renewed membership and named a new chairperson, Julia Fulghum who is a Professor in the Department of Chemistry and Chemical Biology at the University of New Mexico (UNM). She currently serves as Special Assistant to the Dean for Graduate Education in the College of Arts & Sciences.

The current CINT SAC members for 2017 are (new members in bold face):

Barbara Baird, Cornell University
Dimitri Basov, Columbia University



Steve Brueck, Center for High Technology Materials

Juan de Pablo, University of Chicago

Julia Fulghum, *CINT SAC Chairperson*, The University of New Mexico

Rachel Goldman, The University of Michigan

Mark Hampden-Smith, Saint-Gobain Innovative Materials

Rajiv Kalia, University of Southern California

Don Lucca, *CINT UEC Chairperson and ex officio SAC member*, Oklahoma State University

Willie Padilla, Duke University

Andy Shreve, University of New Mexico-Center for Biomedical Engineering

Ting Xu, University of California, Berkeley

- II. Igal Brener, NPON Thrust Co-Leader, gave two invited talks: (1) "All dielectric metasurfaces: enhanced nonlinearities and emission control" at Photonics West on February 1 and (2) "Ultrafast and Nonlinear Metasurfaces" at the 2017 CUDOS Workshop in Australia on February 20.
- III. Igal Brener, NPON Thrust Co-Leader, was issued patent 9,594,266 - Tunable Photonic Device Including an Array of Metamaterial Resonators. The invention relates to photonic devices, and more particularly to optical filters and modulators that incorporate arrays of metamaterial resonators.
- IV. LANL conducts an annual review of its "Materials for the Future" pillar in support of the LANL Strategic Plan. This year the Area of Leadership "Integrated Nanomaterials" is under review, showcasing CINT's capabilities and accomplishments to an external review board and LANL senior leadership. The review will take place May 1-3, 2017.

User Program & Outreach:

- I. CINT has three new leveraged capabilities offered to the user community, one at the Core facility and two at the Gateway. These leveraged capabilities are: (1) Aiping Chen is leading a characterization capability to grow high-quality epitaxial actinide thin films to explore their functional properties and device applications, available at the Gateway. (2) Hou-Tong Chen is leading a scanning near-field microscopy (neaSpec SNOM) capability that enables ~10 nm spatial resolution for mid-infrared (4.6-15.3 μm) spectroscopy and imaging as well as near-infrared-pump/mid-infrared-probe spectroscopy, available at the Gateway. From the Core, (3) Dan Koleske is leading a synthesis and fabrication capability to expand epitaxy for nanoscience using Metal Organic Chemical Vapor Deposition (MOCVD).
- II. CINT co-organized, with CNM, a booth for the APS March Meeting in New Orleans, March 13-16, 2017. The joint NSRC booth was staffed by: Julie Emery (CNM), Grace



Webster (CFN), Heather Brown (CINT), and Cathy Jo Beecher (CINT). We recorded over 230 researchers at the booth. Combined, the NSRCs represented over 100 talks and poster presentations at the meeting.

- III. CINT Gateway hosted a tour of ten students from Johns Hopkins Society of Physics on March 24.
- IV. CINT Spring call for proposals is open March 1-31, 2017. Proposals accepted during this call will be active July 1, 2017 – December 31, 2018.

News:

- I. Brian Swartzentruber, former CINT NEM Thrust leader, has been hired as the manager of organization 1132, the Nanosystems Synthesis and Fabrication organization at Sandia National Laboratories within the CINT organization.
- II. Nate Mara, former NEM Thrust Co-Leader, will succeed Brian as NEM Thrust leader. Mike Lilly will serve as the NEM Thrust Co-Leader.
- III. Jim Werner, CINT scientist, has been named as acting Los Alamos CINT Group Leader. Jeff Willis, from Los Alamos MPA-11, is currently serving as acting Deputy Group Leader.
- IV. LANL conducts an annual review of its “Materials for the Future” pillar in support of the LANL Strategic Plan. This year the Area of Leadership “Integrated Nanomaterials” is under review, showcasing CINT’s capabilities and accomplishments to an external review board and LANL senior leadership. The review will take place May 1-3, 2017.
- V. CINT has been engaged in the transition of Sandia’s Management & Operations contract from Lockheed Martin to National Technology and Engineering Solutions of Sandia (NTESS) a wholly owned subsidiary of Honeywell. These activities have included a 3-hour review of the CINT program at Sandia and a 2-hour safety walk-through of the CINT Core.

Budget

- I. Please see attached [NSRC_CINT_Monthly_Budget_March_2017.xlsx](#) for 1-yr projections and March 2017 monthly breakdown.
- II. New spreadsheet reports at the program level. Previous report had a cost by thrust breakdown.
- III. The line item highlighted in peach titled “AIP & Equipment Plan” represents our recap expenditures.